

IQI 04, Seminar 13

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- Quantum physics simulation.

E. “Manny” Knill: knill@boulder.nist.gov

Quantum Physics Simulation

- Superficial problem statement.

Given: A model of a quantum physics system.

Problem: Determine a physical quantity.

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- Example models.
 - A particle of mass m in one dimension.
 \mathcal{H} : Square integrable functions on $\mathbb{R} = (-\infty, \infty)$.
$$H = -\frac{1}{m}\frac{\partial^2}{\partial x^2} + V. \quad [\dots \hbar = 1]$$

Unitary evolution according to Schrödinger's equation:
$$\frac{\partial}{\partial t}\psi = -iH\psi.$$

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- N particles in 3 dimensions.

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- Translation invariant 1-D lattice of spin- $\frac{1}{2}$ systems.

$$H = \sum_k H_I^{(k,k+1)}, \text{ with } H_I^{(k,k+1)} = \sum_{u,v} \alpha_{u,v} \sigma_u^{(k)} \sigma_v^{(k+1)}$$

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[“virtual” experiment is q. easy]



Physics Simulation Algorithms: Common Features

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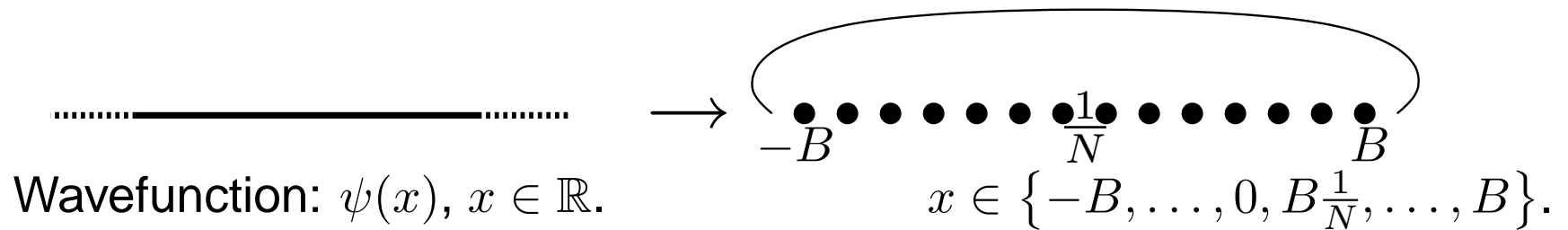
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Wavefunction: $\psi(x)$, $x \in \mathbb{R}$.



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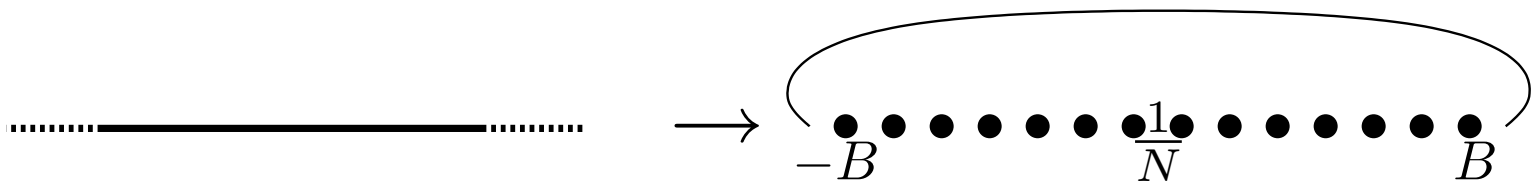
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$\sum_x \frac{1}{m} F x^2 |x\rangle \langle x| F^\dagger + V(x) |x\rangle \langle x|$
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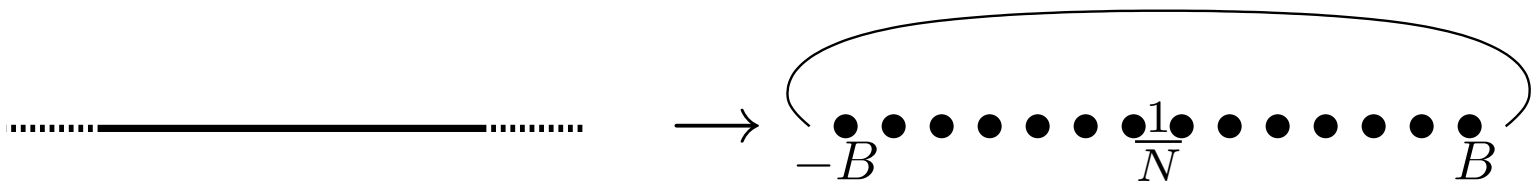
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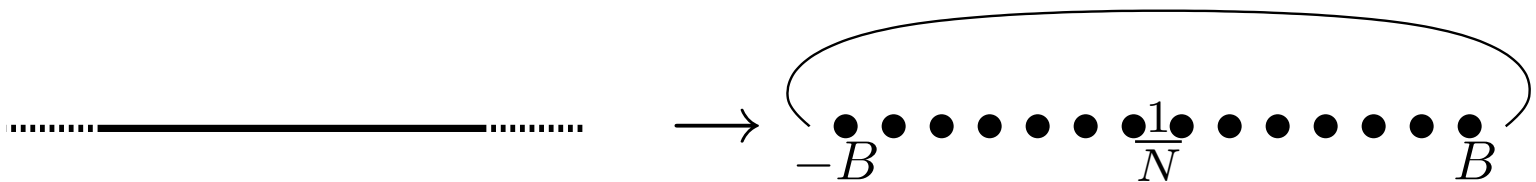
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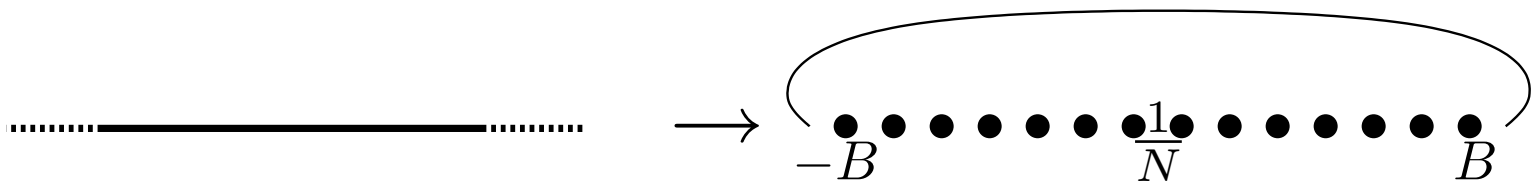
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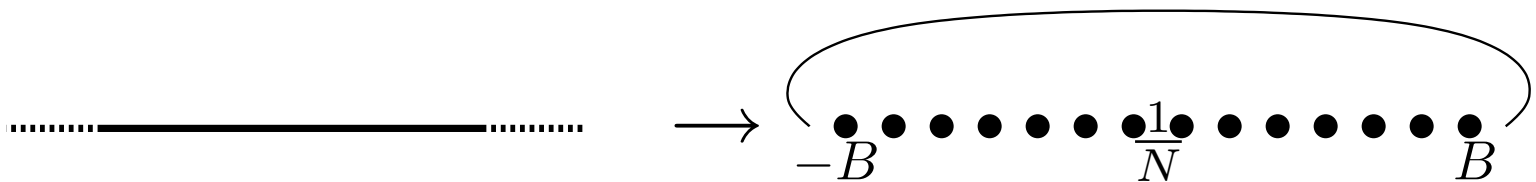
- $\mathbf{K} = F \sum_x \frac{1}{m} x^2 |x\rangle \langle x| F^\dagger$, $\mathbf{V} = \sum_x V(x) |x\rangle \langle x|$.

Trotterization: $e^{-iHt} = (e^{-i\mathbf{K}t/T} e^{-i\mathbf{V}t/T})^T + O(1/T)$



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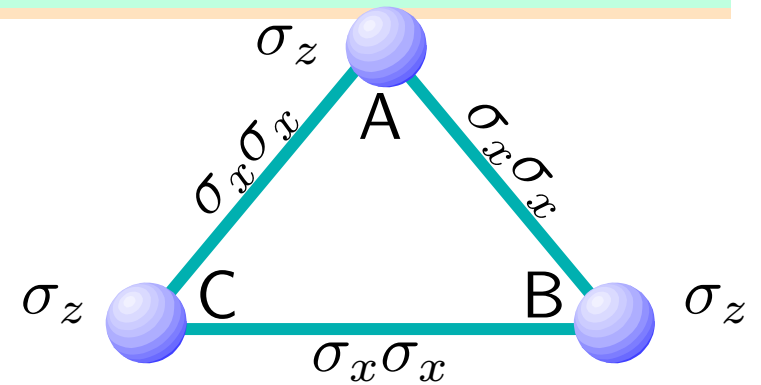
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- Information extraction: State preparation and measurement.



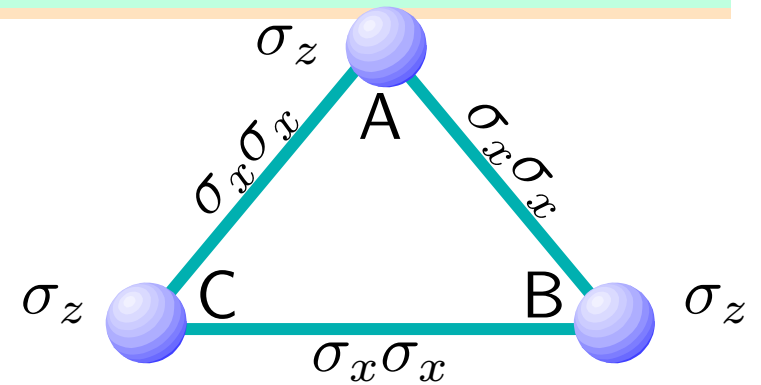
Faithful Evolution

- Example: Triangle XY -model.



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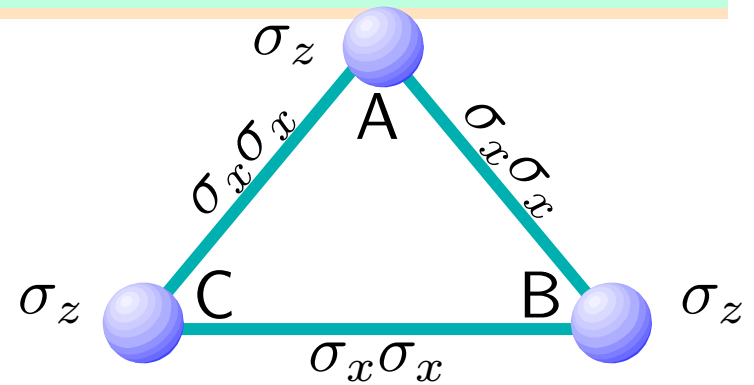
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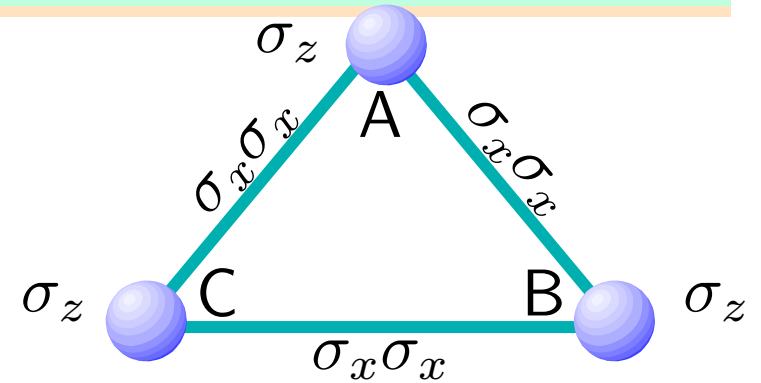
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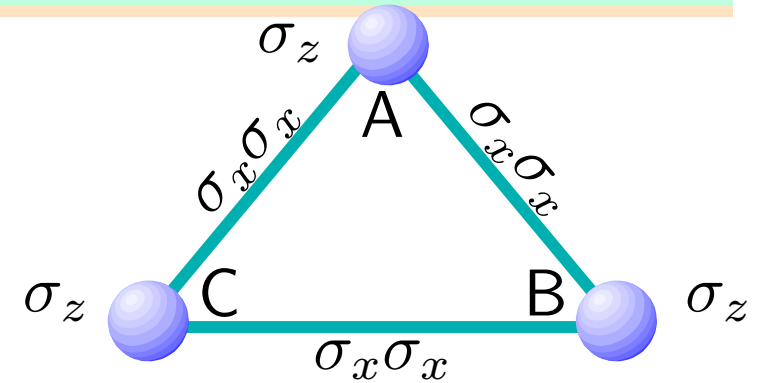
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$e^{-i\sigma_z^{(U)} t}$: A z -rotation. 




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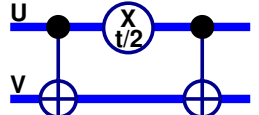
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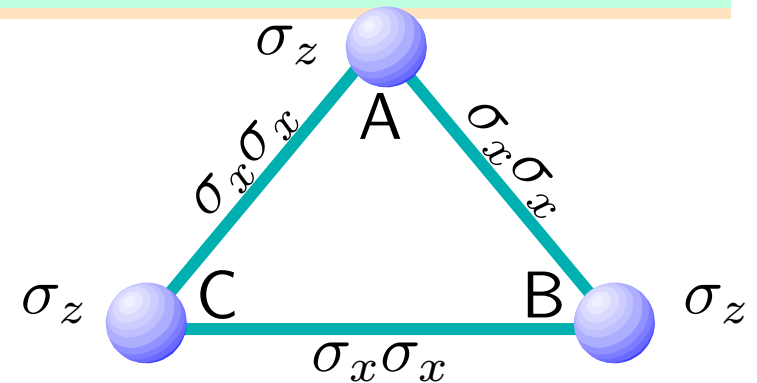
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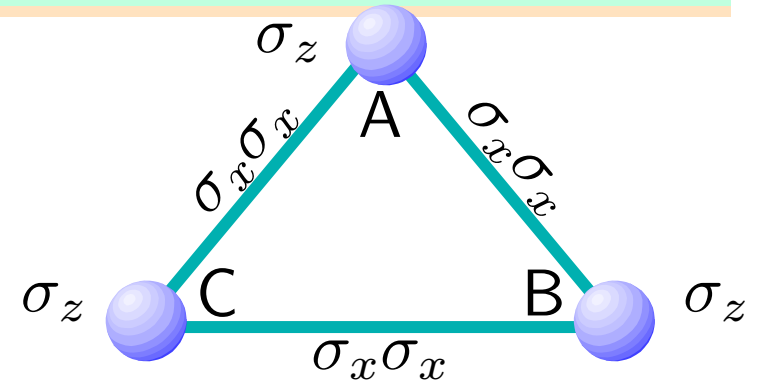
$$H_{int} = \sigma_z^{(A)} + \sigma_z^{(B)} + \sigma_z^{(C)}, H_{cpl} = \sigma_x^{(A)} \sigma_x^{(B)} + \sigma_x^{(A)} \sigma_x^{(C)} + \sigma_x^{(B)} \sigma_x^{(C)}.$$



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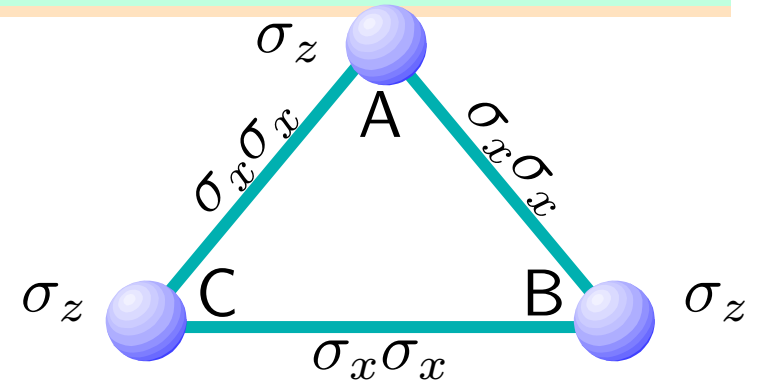
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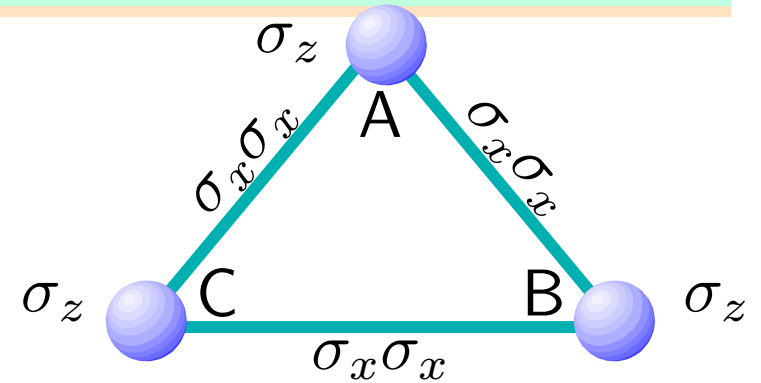
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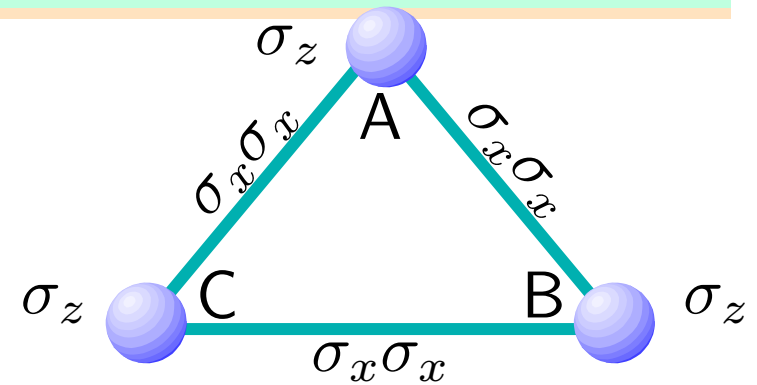
Trotterize: $e^{-iHt} = e^{-i(H_{int}+H_{cpl})t}$



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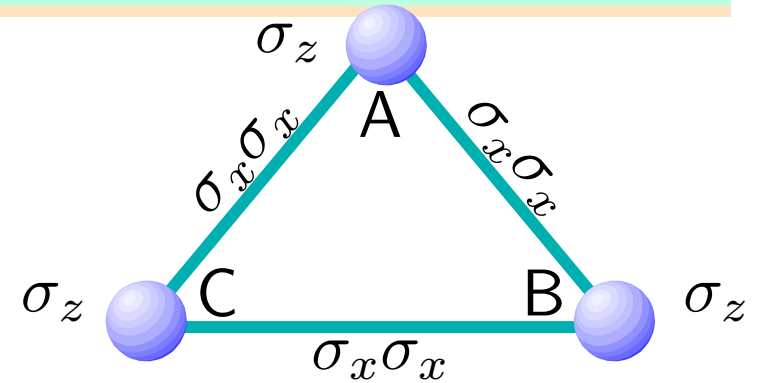
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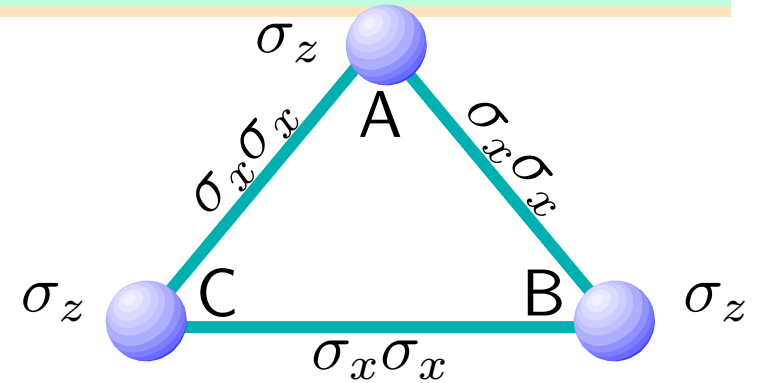
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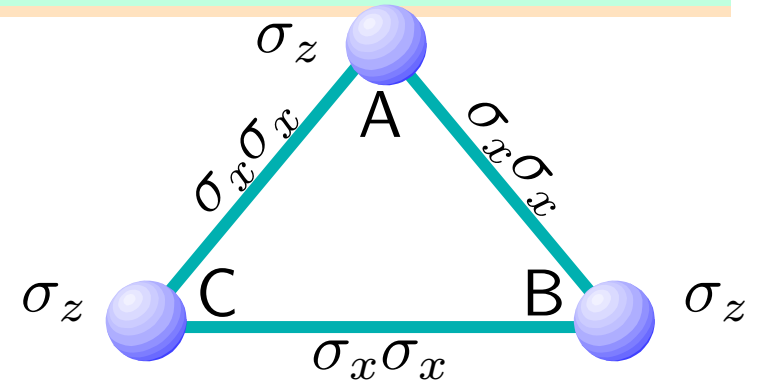
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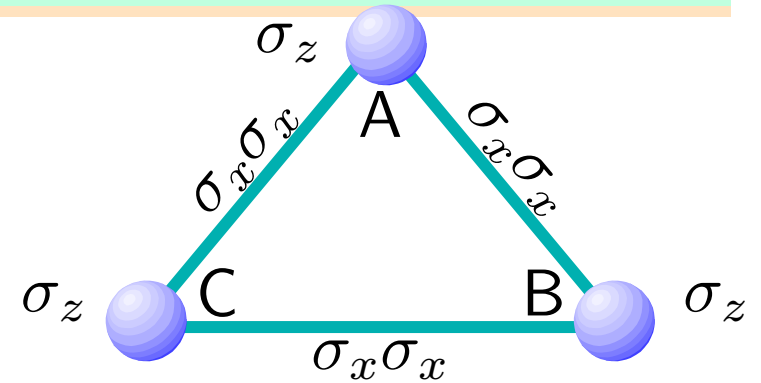
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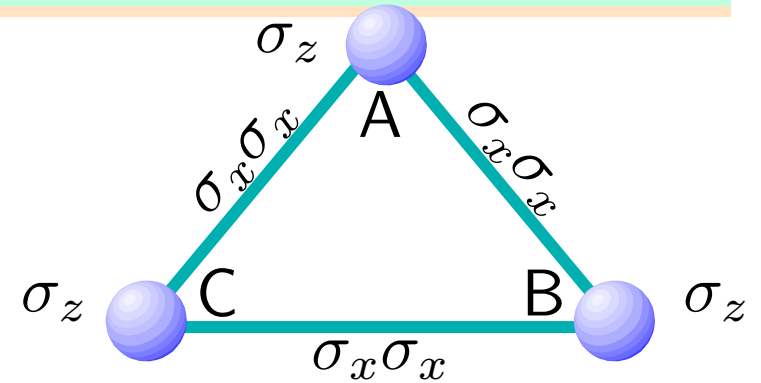
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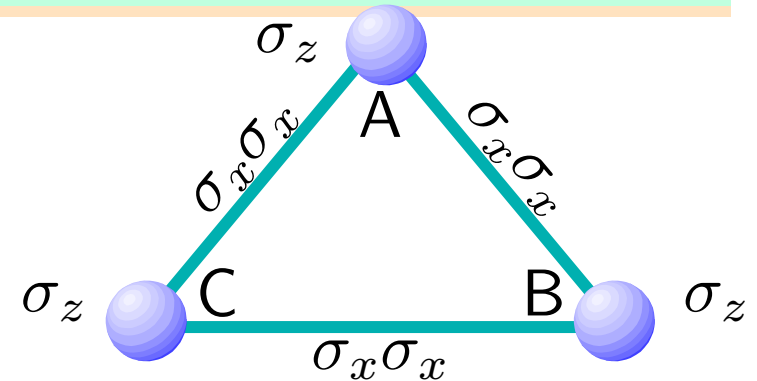
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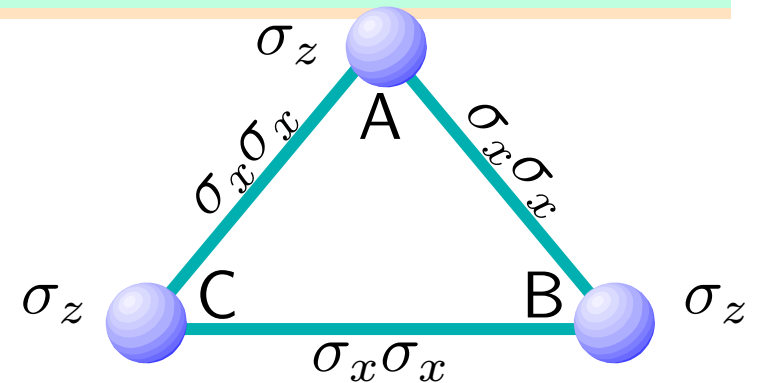
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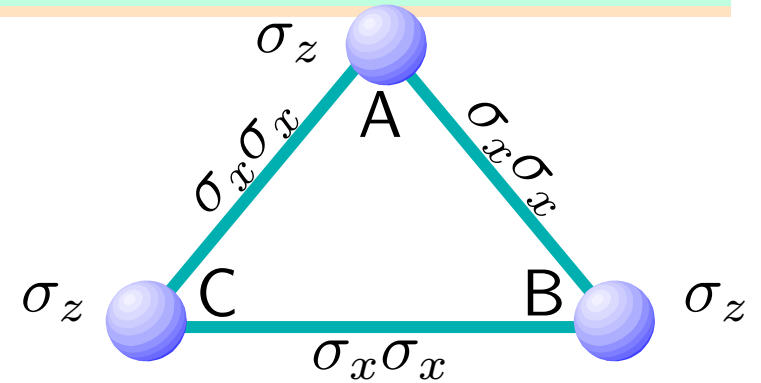
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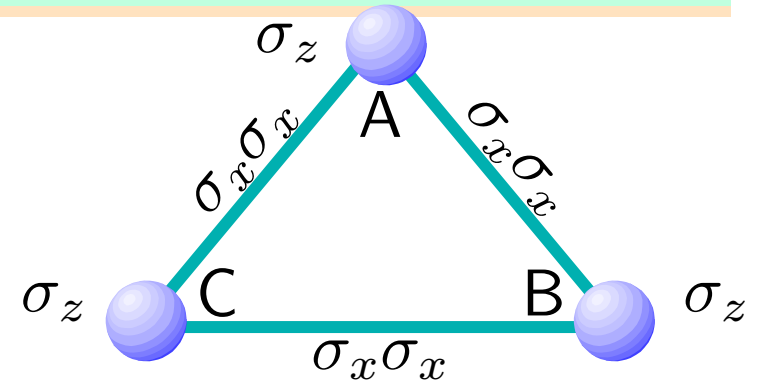
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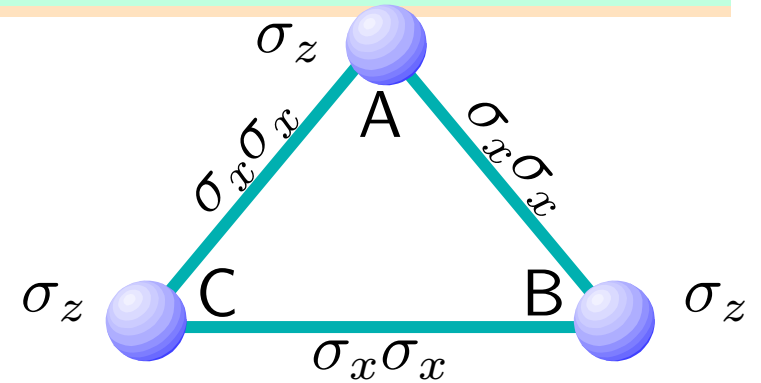
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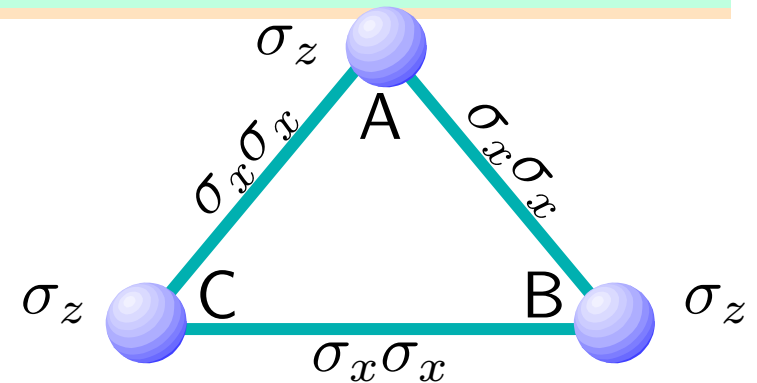
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But the terms do not all commute. Combine commuting terms:

$$H_{int} = \sigma_z^{(A)} + \sigma_z^{(B)} + \sigma_z^{(C)}, \quad H_{cpl} = \sigma_x^{(A)} \sigma_x^{(B)} + \sigma_x^{(A)} \sigma_x^{(C)} + \sigma_x^{(B)} \sigma_x^{(C)}.$$

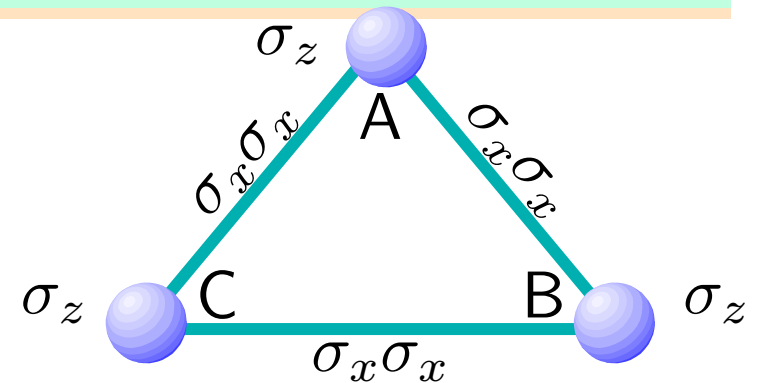
$$e^{-iH_{int}t} = e^{-i\sigma_z^{(A)} t} e^{-i\sigma_z^{(B)} t} e^{-i\sigma_z^{(C)} t}, \text{ similarly for } e^{-iH_{cpl}t}.$$

$$\text{Trotterize: } e^{-iHt} = \left(e^{-iH_{int}\frac{t}{N}} e^{-iH_{cpl}\frac{t}{N}} + O((|H|\frac{t}{N})^2) \right)^N$$



Faithful Evolution

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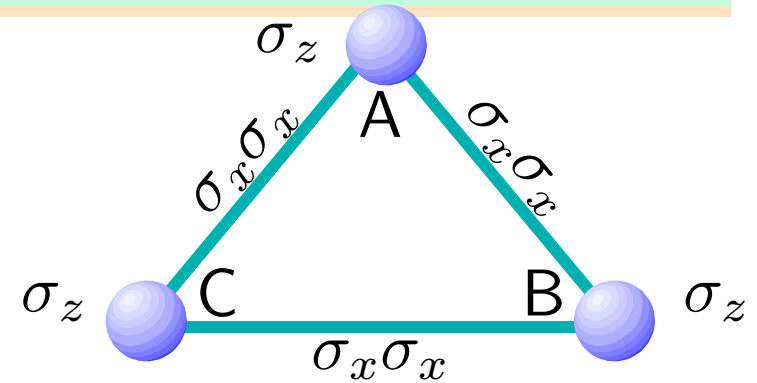
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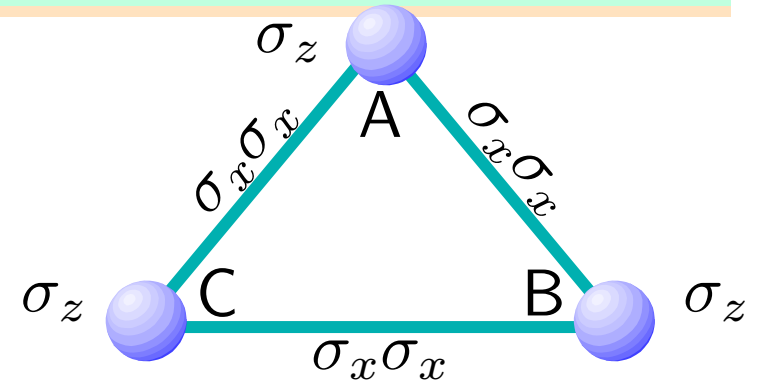
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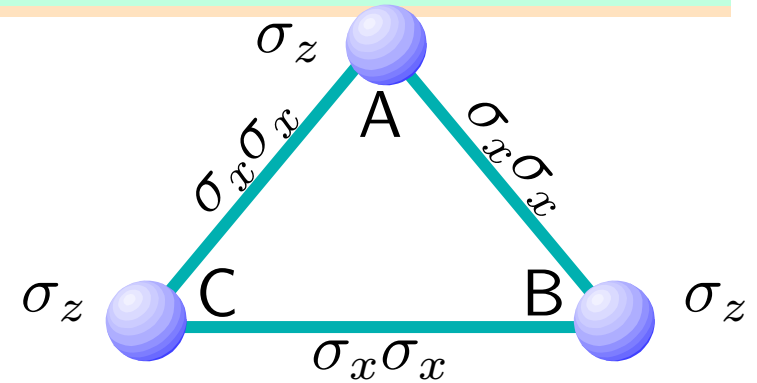
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Simulatability of Physical Systems

Physical universality thesis for quantum computers.

Given: Physical system S .

Physical Hamiltonian $H \geq 0$ for S .

Physically meaningful state $|\psi\rangle$ of S of av. energy E .

Then: It is possible to represent S , H and $|\psi\rangle$ on qubits,
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The Virtual Quantum Physics Lab

- Quantum computers can efficiently simulate an experimental procedure on a specified quantum system.



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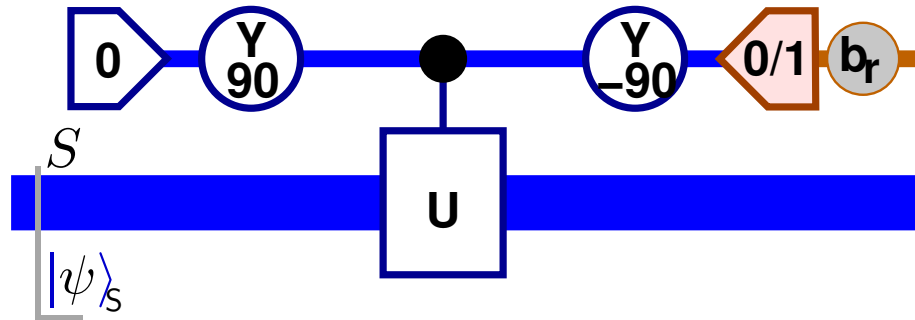
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Problem: Measure $\langle\psi|U|\psi\rangle$ to within ϵ .



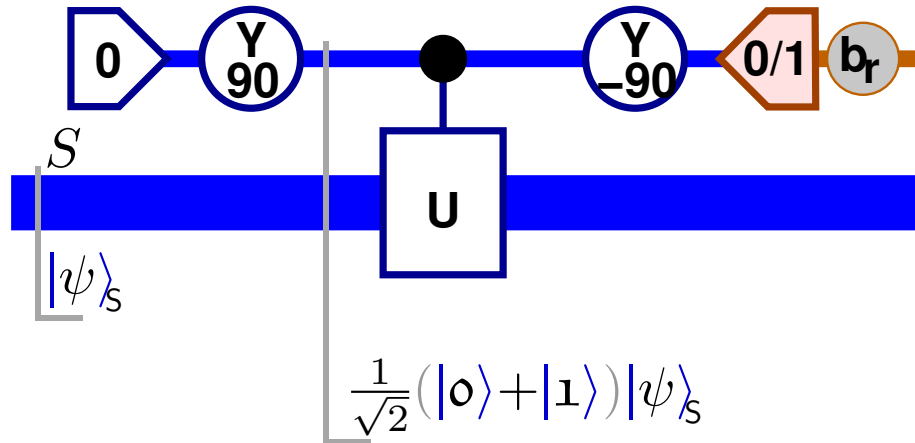
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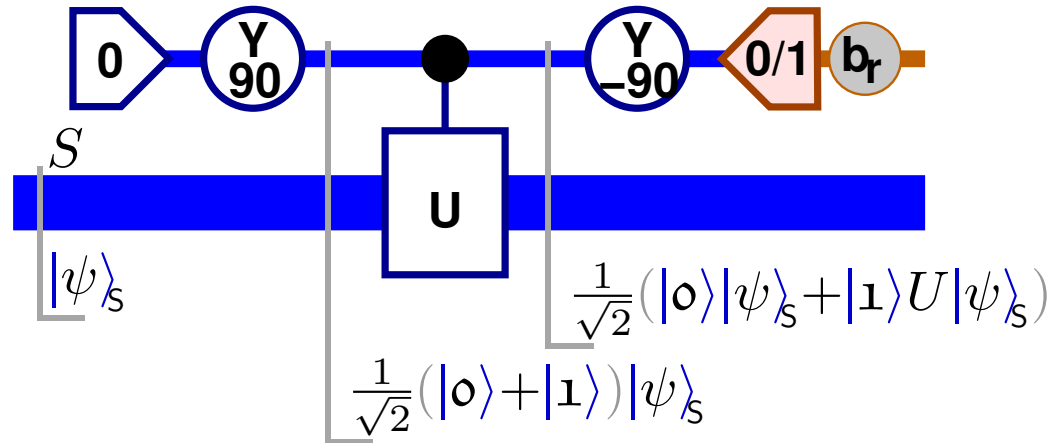
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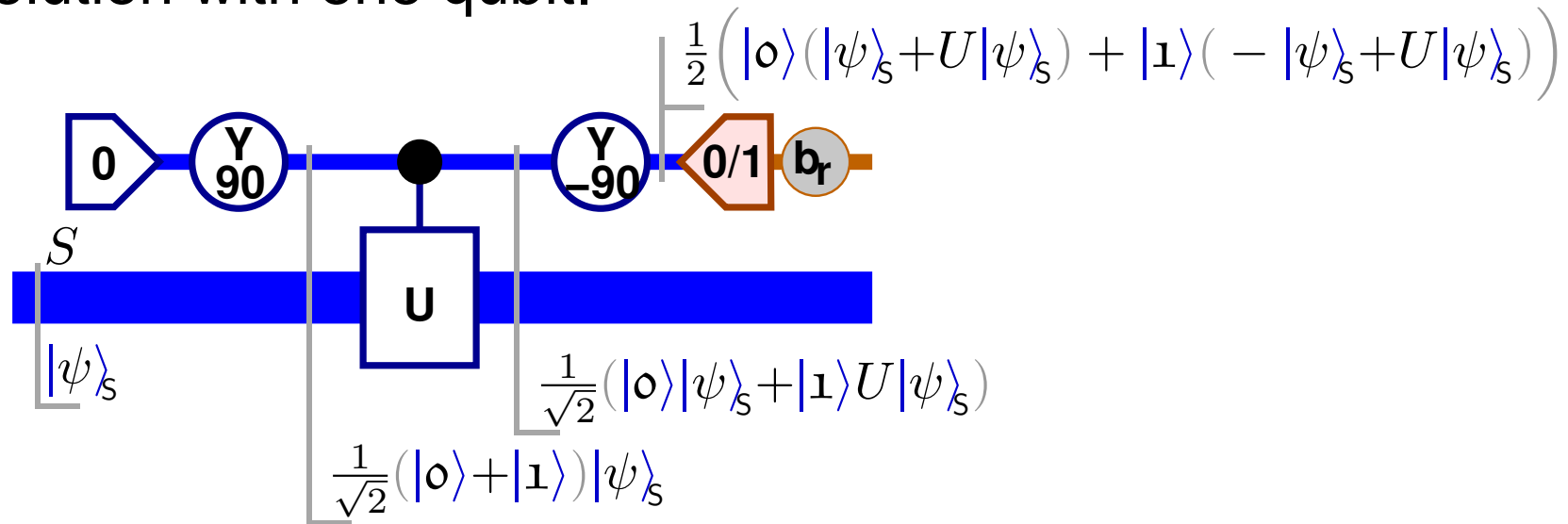
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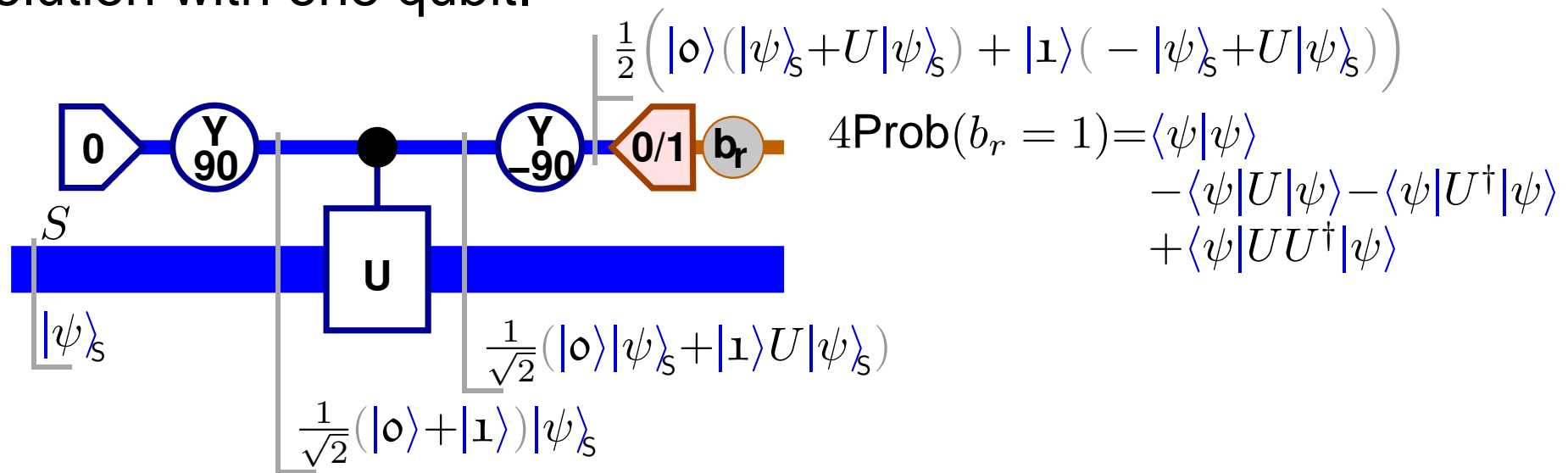


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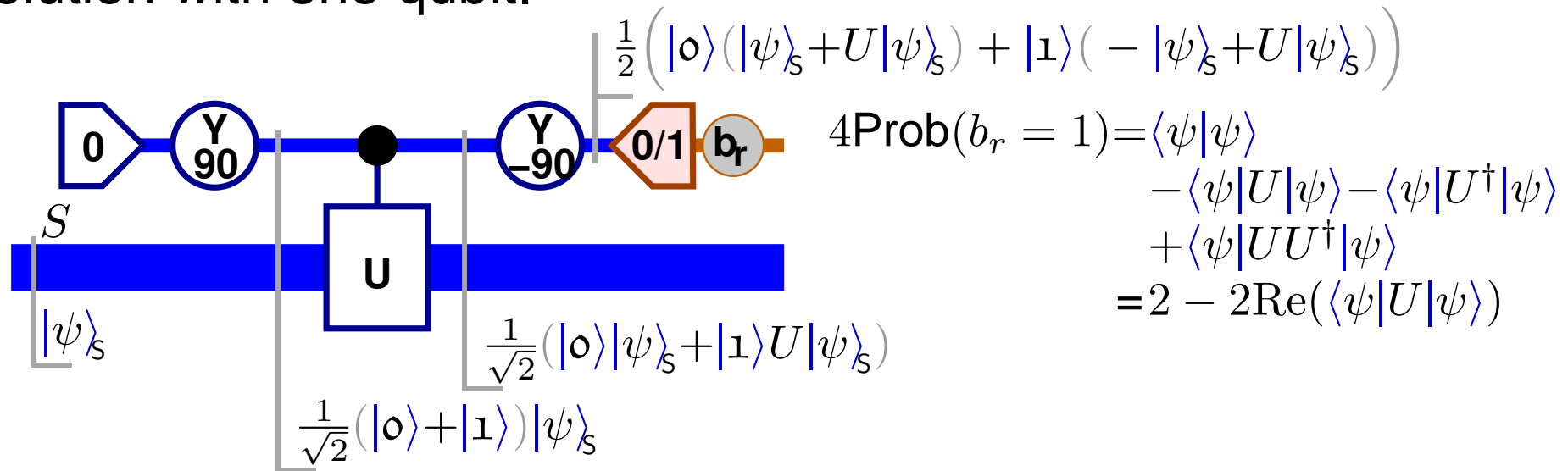


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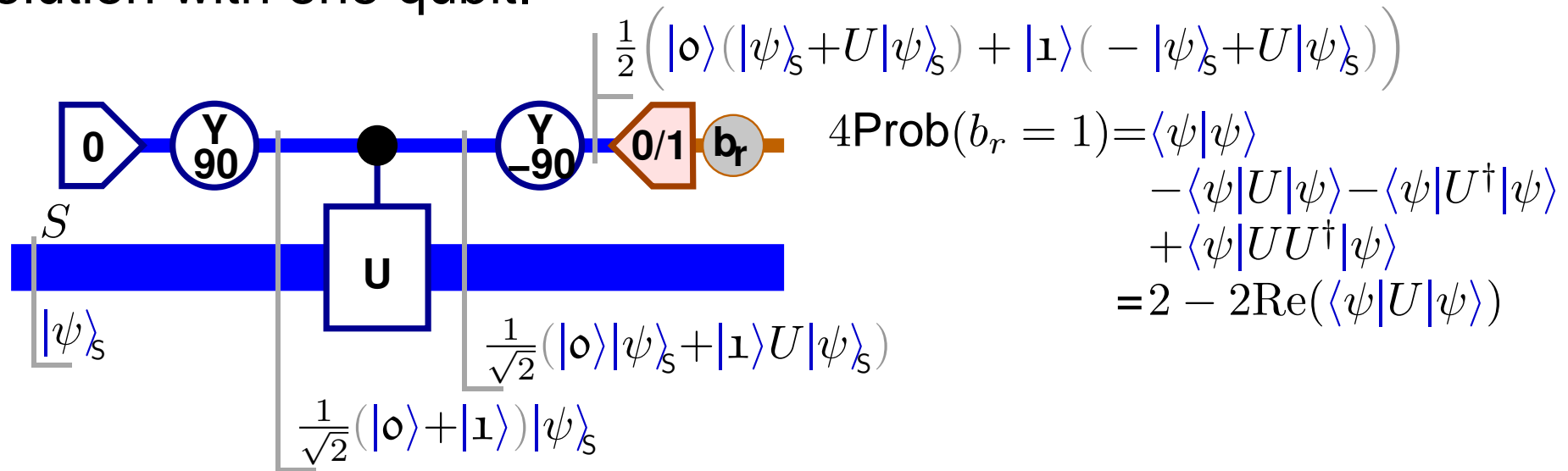


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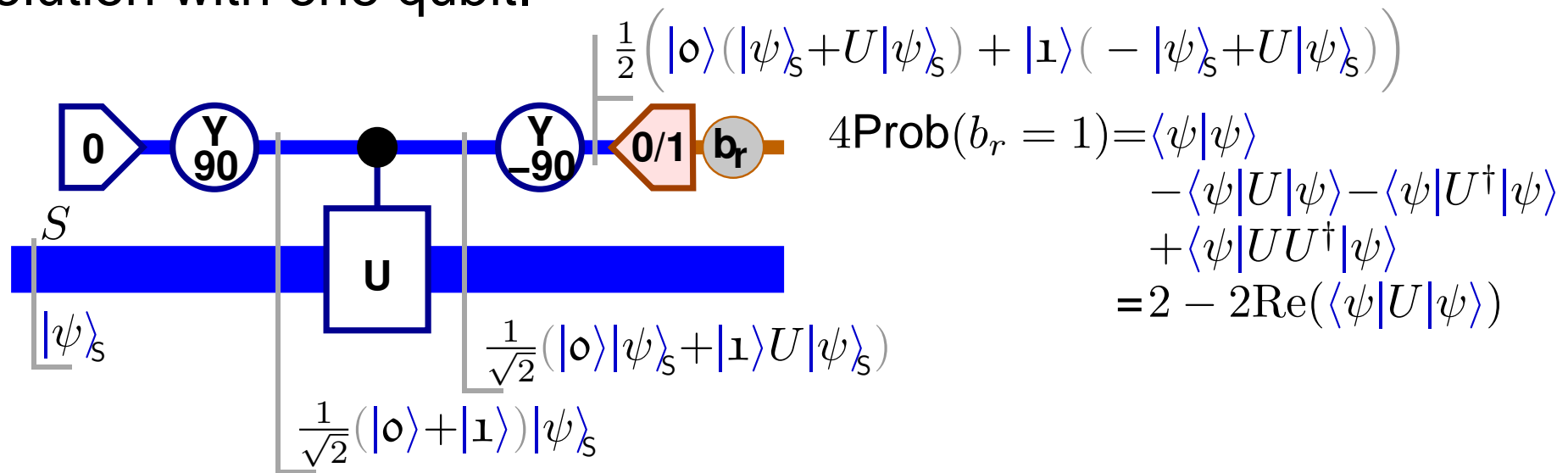
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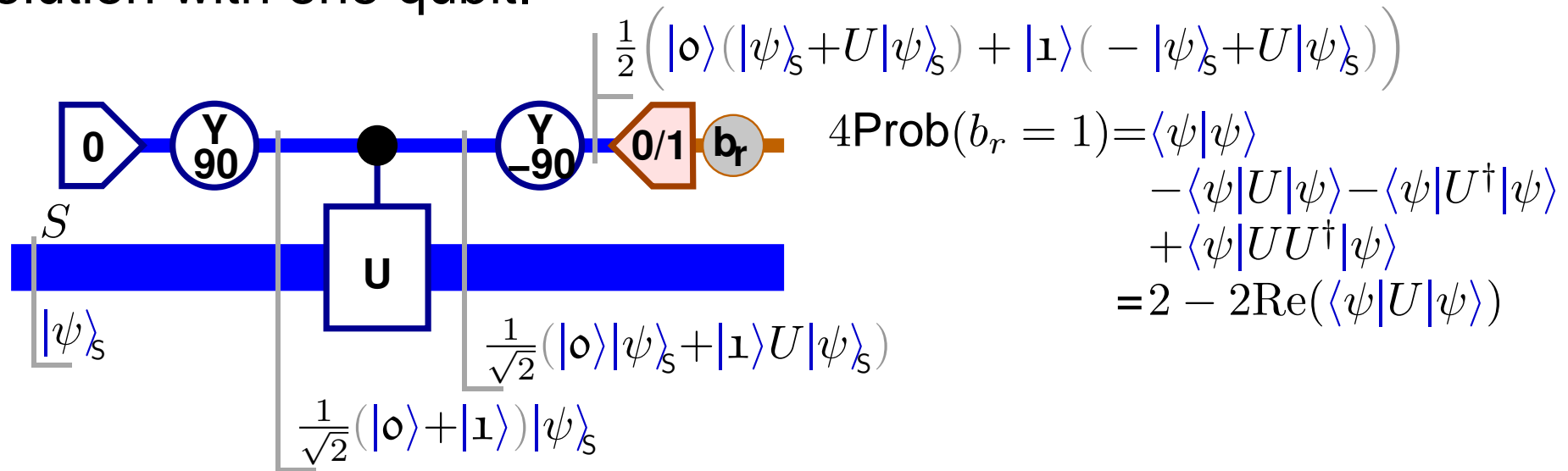
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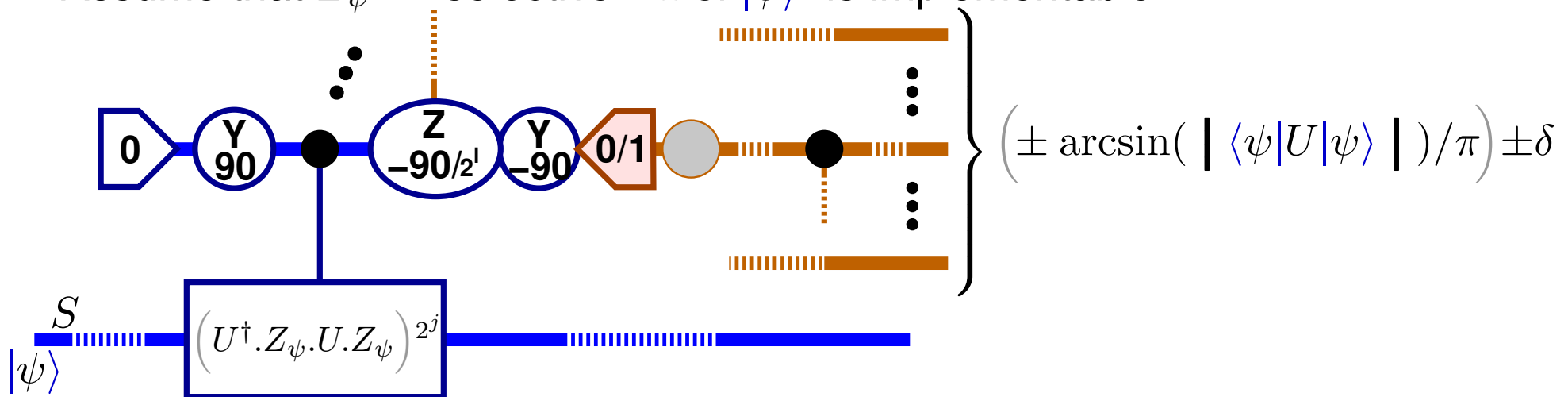
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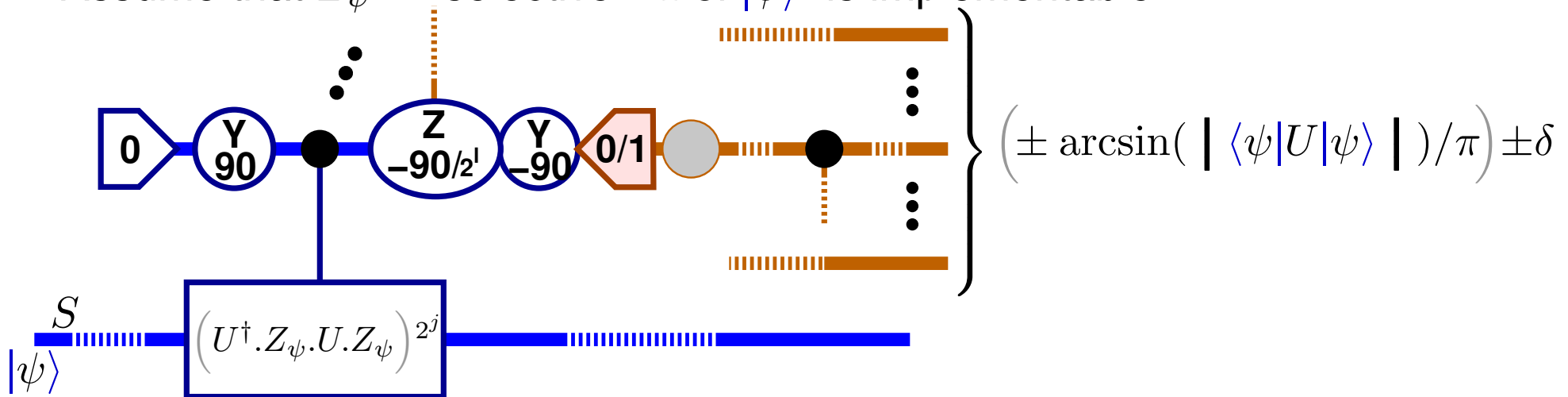
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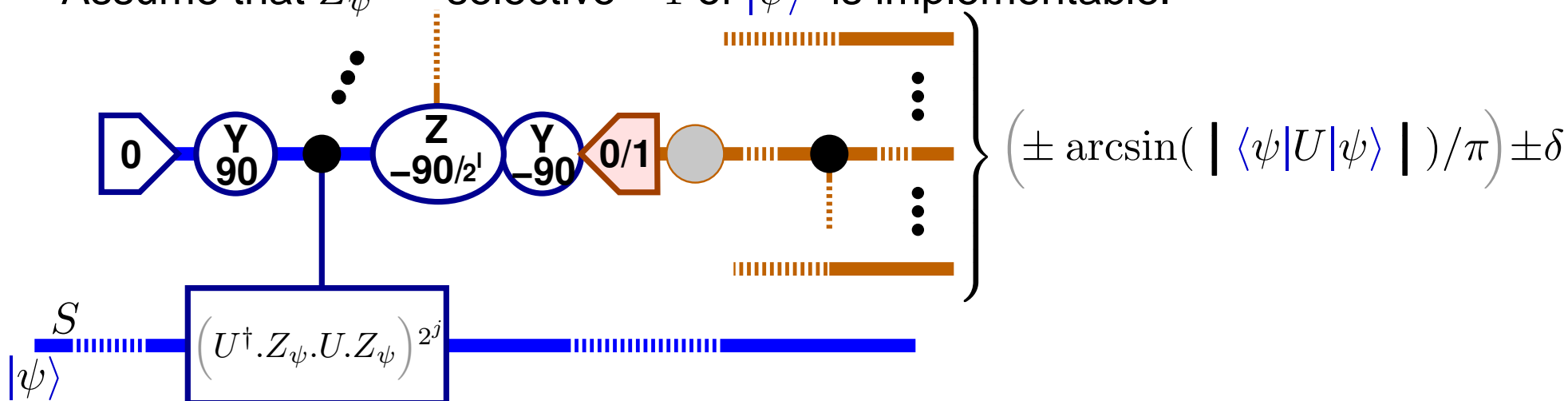
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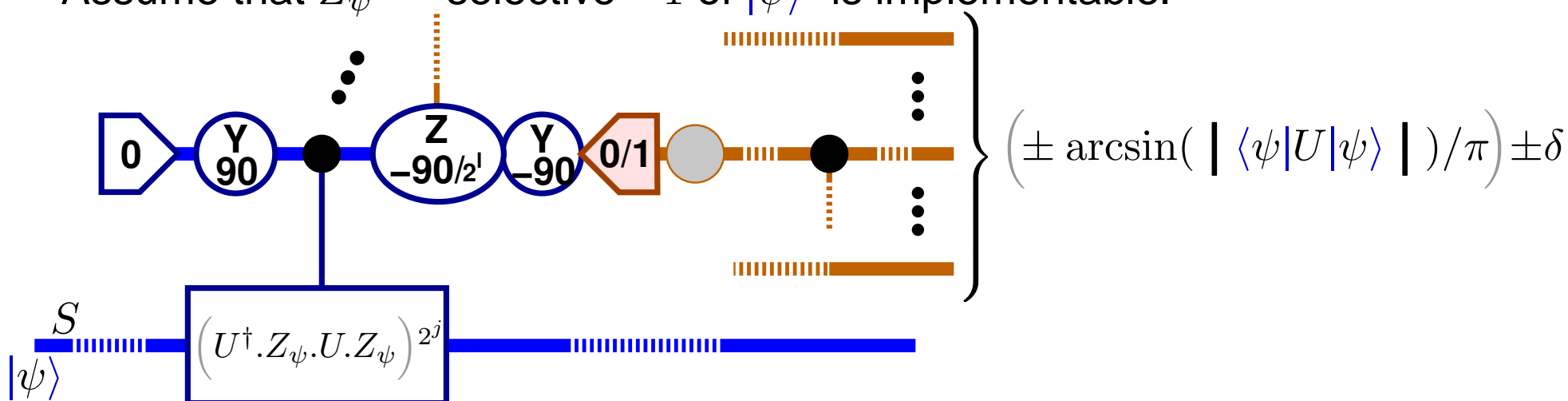
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– Requires $O(1/\epsilon)$ coherent, controlled applications of U .

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 - For small t , $e^{-iAt} = 1 - itA + O(|A|^2t^2)$.
$$\langle\psi|e^{-iAt}|\psi\rangle = 1 - it\langle\psi|A|\psi\rangle + O(|A|^2t^2)$$
 - Choose t such that $O(|A|^2t^2)$ contributes at most $t\epsilon/2$.
$$t = O(\epsilon/|A|^2)$$
 - Measure $\langle\psi|e^{-iAt}|\psi\rangle$ to within $t\epsilon/2$.
- Requires $O(|A|^2/\epsilon^2)$ uses of e^{-iAt} with amp. estimation.



Measuring Correlation Functions

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Operators A and B , implementable as needed.
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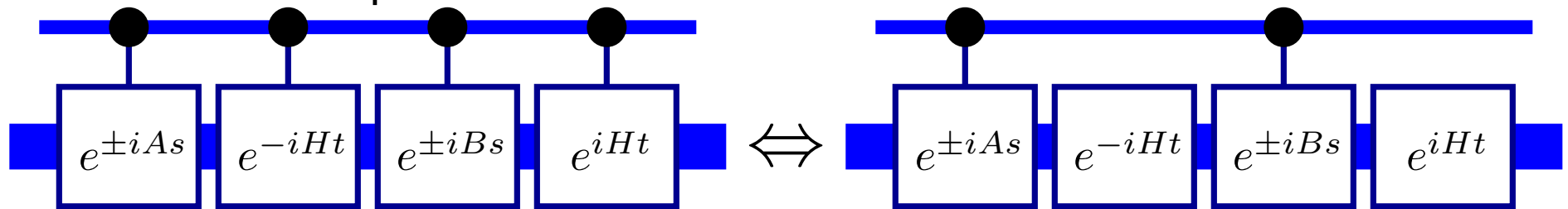
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- Note network simplification:



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- Requires $O(|H|S/\epsilon)$ uses of e^{-iHt} with t up to $O(1/\epsilon)$.



State preparation Problems

- Prepare the ground state of H ?



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... can simulate contact with a thermal bath, but efficiency?



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